Performance Portability Experiences & Challenges in Lattice QCD

Bálint Joó, Jefferson Lab
discussing also the work of others: P. Boyle (U. Edinburgh), K. Clark (NVIDIA), R. Edwards (JLab), J. Osborn (ALCF), F. Winter (JLab) and S. Khan (ODU) with help from C. Trott (Sandia)

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- Bespoke Performance Libraries
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  - QDP-JIT for CPUs and GPUs
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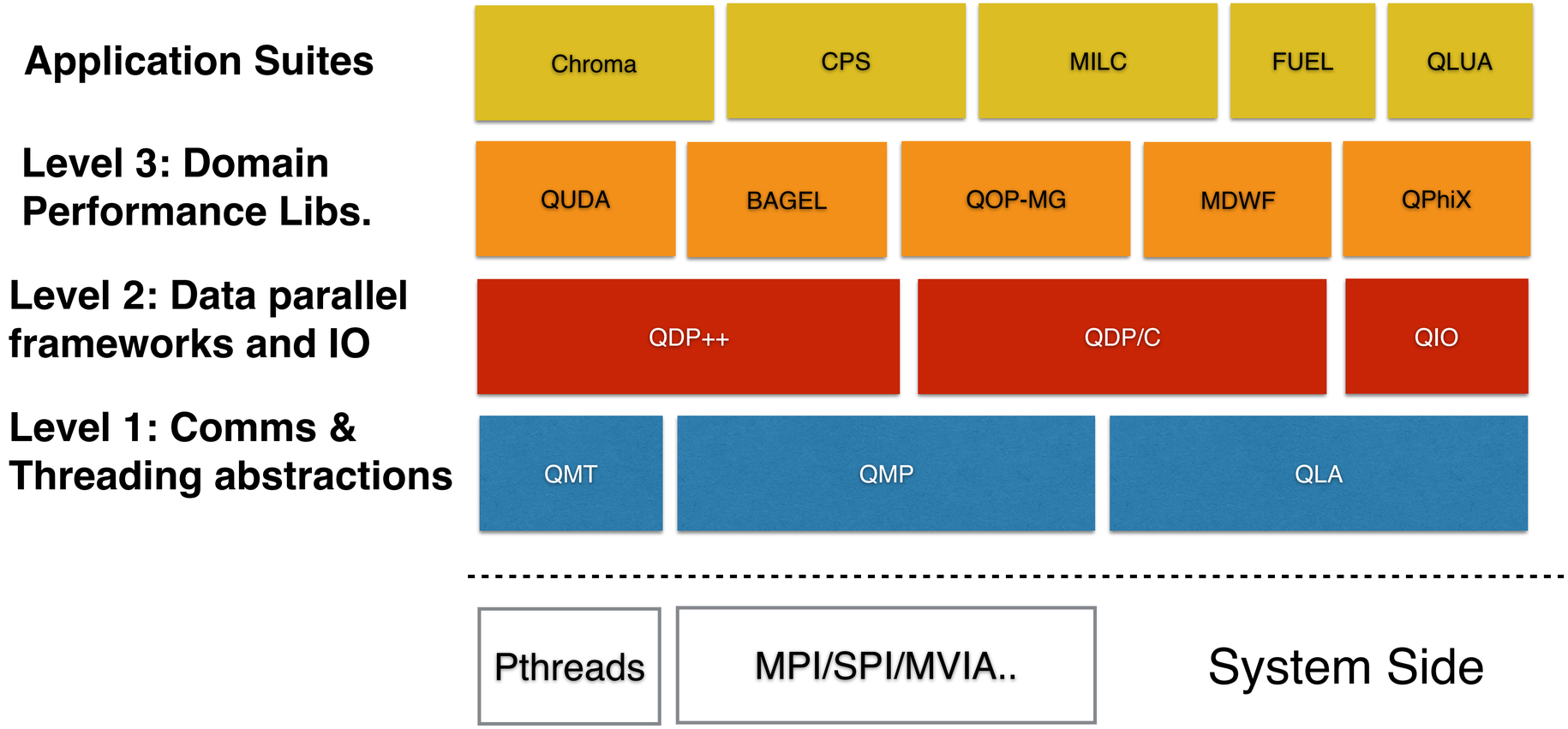
  - QEX
- Very recent Kokkos experience
- Lessons Learned

This is a review-like talk, I didn't do all the work. All mistakes/errors etc. about work of others are mine.

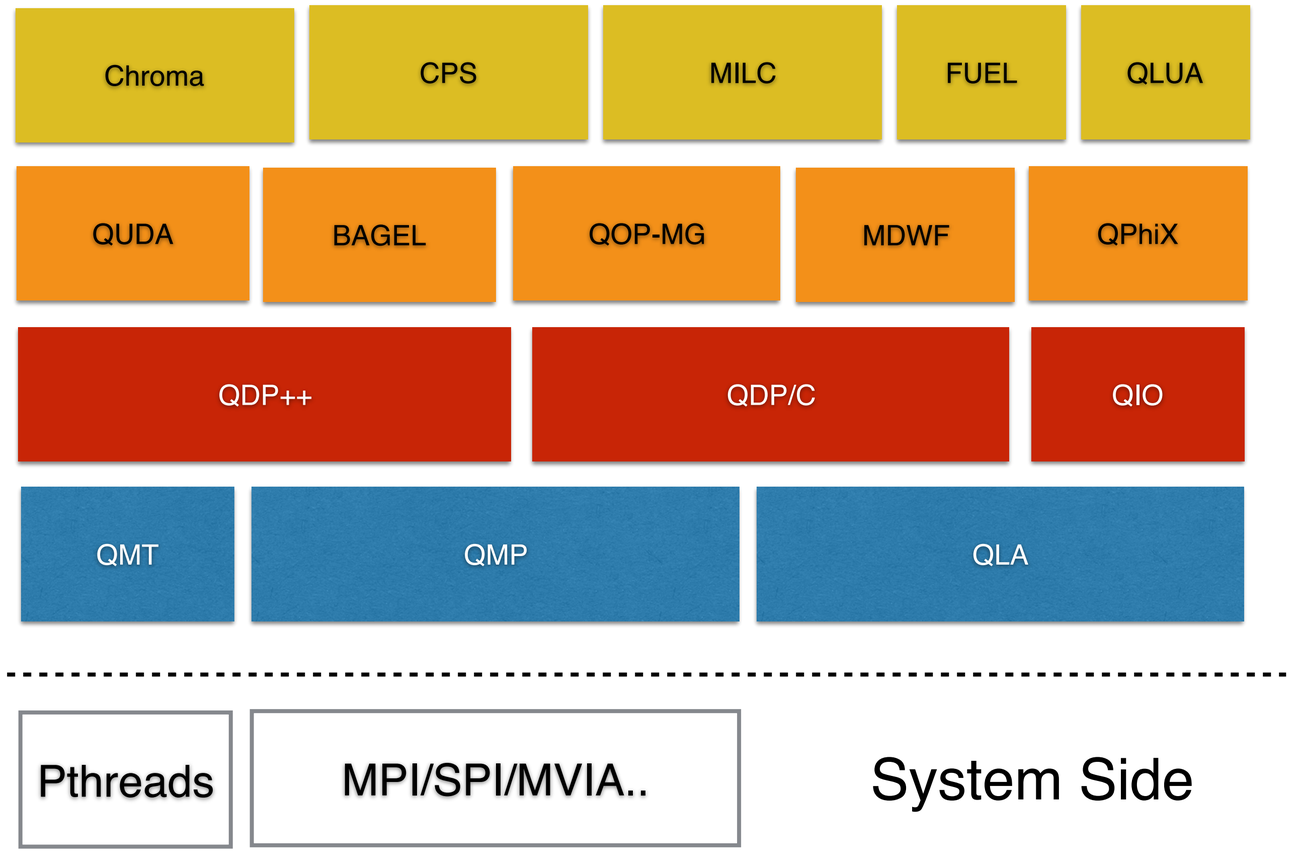
USQCD SciDAC Layered Software



- Layered approach
- Performance libraries - tied to architecture
- Data parallel frameworks for productivity
- Wrap MPI etc.

Pros and Cons

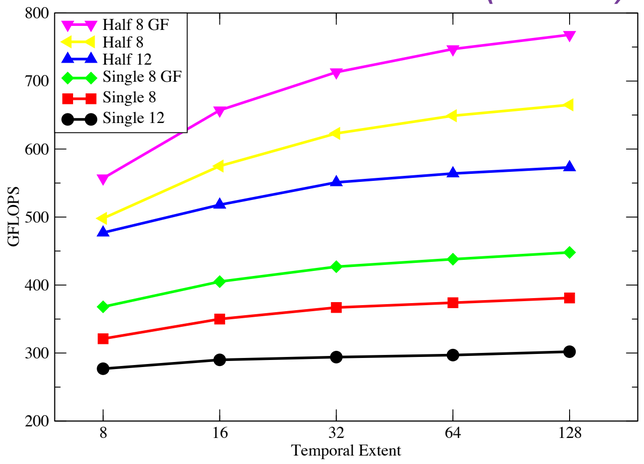
- “Performant Capability Portability”
  - but only as long as capability is provided in Level 3 libraries for all architectures of interest
  - Libraries often compete, features not always in sync
- Good reuse of libraries between applications (e.g. QUDA)
- Has been ‘very portable’
  - QCDOC, Cray XT, XE and BlueGene systems, Xeon Clusters
- Level 2 data layouts have not been flexible, and have typically been AOS. Difficult to vectorize
  - libraries require data import/export, need to be sufficiently granular to amortize this
  - ‘native’ level 2 code, can become Amdahl’s law bottleneck

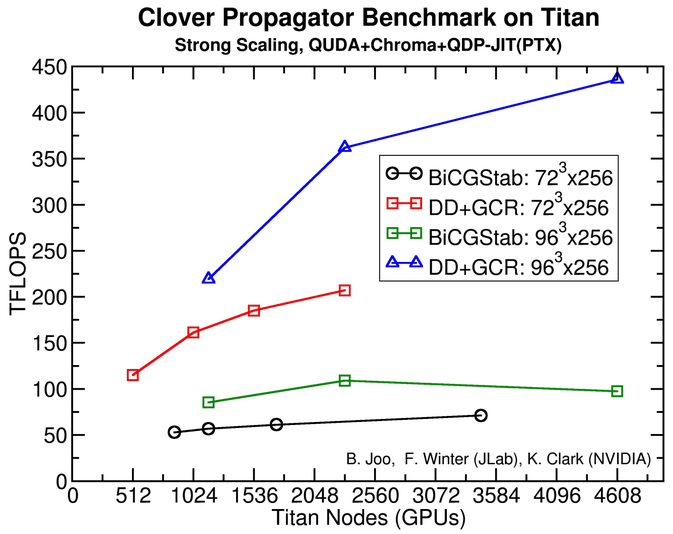


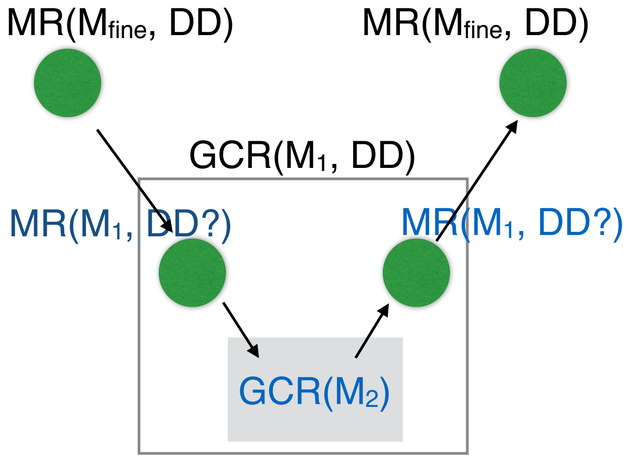
Domain Specific Performance Libraries

- Great way to learn about the architectures
- QUDA for GPUs:
  - vital importance of data layout
  - use of mixed precisions
  - use of compression
  - use scalable methods!
  - CUDA C++ based.
- Bagel and QPhiX libraries for multicore CPUs
  - AOS/SOA/AOSOA layouts
  - cache-blocking approaches
  - load-balancing / prefetching
  - Intrinsics + OpenMP/pthreads based (QPhiX), assembler (BAGEL)
- Very suitable for ‘simple’ solvers (CG & BiCGStab)
- ***Complicated solvers (e.g. multilevel AMG) painful***
  - ***need to refactor library into a framework: e.g. QUDA***

K. Clark - GTC 2016 (K20X)





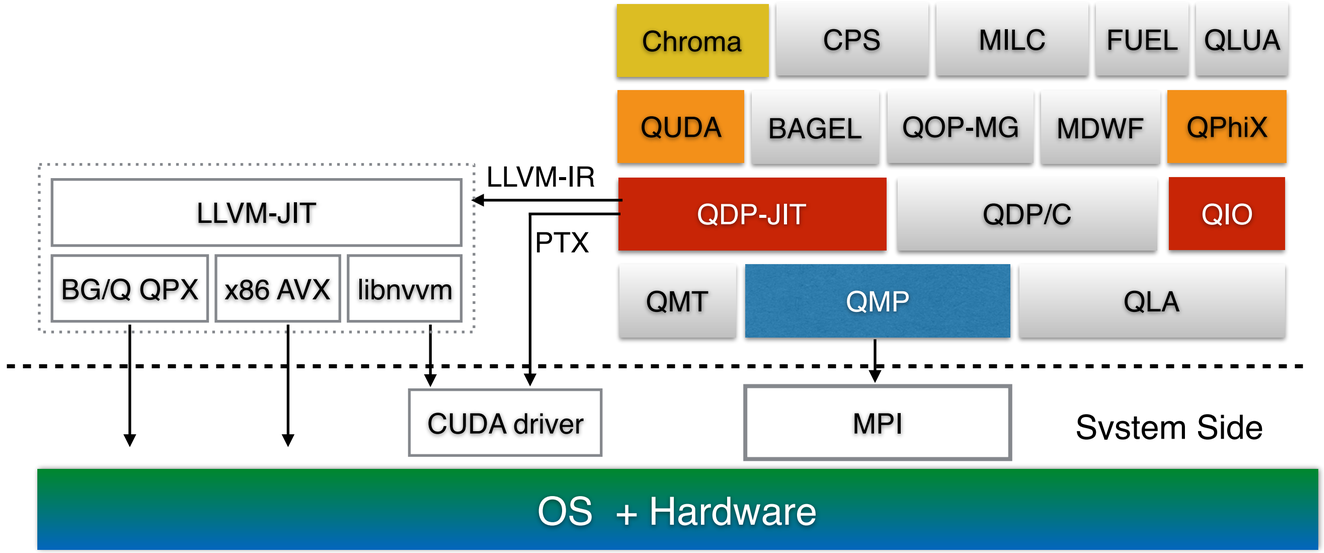


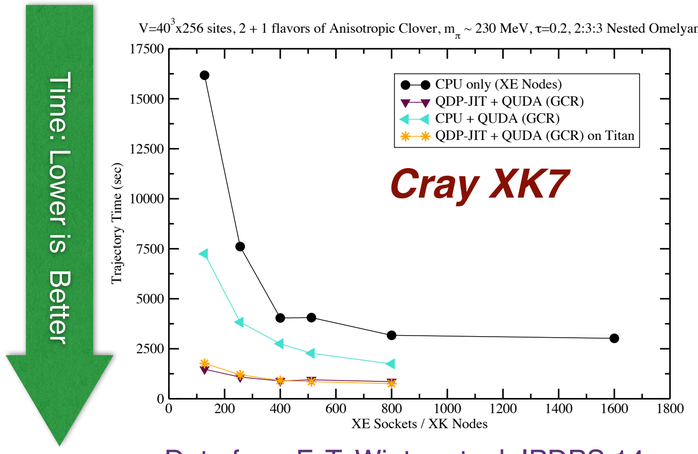
Vcycle Preconditioner:

- multiple solvers,
- indexing multiple lattices
- different operators
  - fine, fine DD?
  - coarse, course DD?
- change layout per level?
- where do grids live?
- where do levels execute?
  - CPU or GPU?

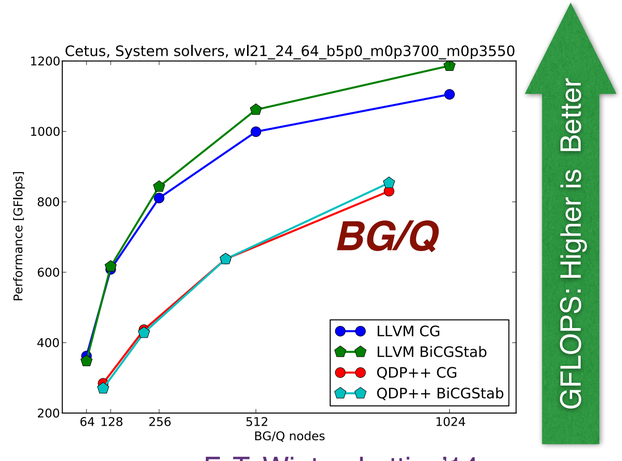
Extreme Metaprogramming I: QDP-JIT

- QDP-JIT
  - Subvert PETE expression templates in QDP++ to produce Just In Time Code Generators
  - Produce PTX (initially) or LLVM-IR (now)
  - Use LLVM optimization passes
  - Use LLVM back end to target hardware
- Drop in replacement for QDP++
  - Deploy all of Chroma on GPUs as well as CPUs
- Divorce data layout from QDP++ data structures
  - different (good) layouts on GPU & CPU
- Treat GPU memory as LRU cache
  - Cache management via CUDA for GPU
  - Could generalize to other Slow/Fast memory combinations.
- Downsides:
  - JIT Overhead: no problem for long duration jobs
  - Dependent on LLVM and PTX versions potentially
  - Maintainance/extension needs LLVM expertise





Data from F. T. Winter et. al. IPDPS 14



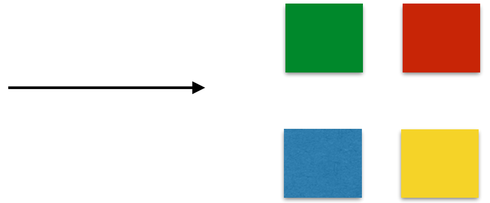
F. T. Winter, Lattice'14

Extreme Metaprogramming II: Grid

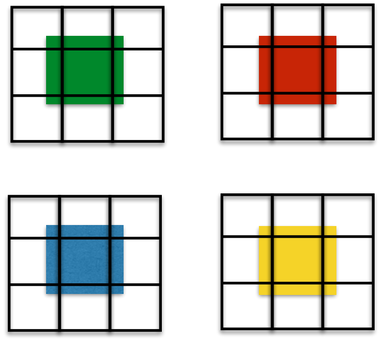
- Recent development from University of Edinburgh (P. Boyle)
  - Address performance concerns of native (non-JIT) QDP++
  - Add multi-level features
  - Emphasis on Data Layout
  - Use virtual node idea from Connection Machine days
  - Solve problem of ‘vectorization’, can work for GPU Warps too.
- Uses C++-11 features for metaprogramming
  - decltype, constexpr etc.
  - smaller code than PETE
  - multi-resoluton ideas (generic forall)
  - comms optimization (e.g. stencil concept)
- Performance is key
  - “Designed to ONLY use and propagate vector intrinsics globally throughout data parallel code: wrapped in high level operators and each defined precisely once in a single short (400LoC) file making porting exceedingly easy”
- Not yet portable to GPUs
  - Future goal: using evolutions of OpenMP offload/OpenACC
  - Combining directives with metaprogramming can be tricky: R&D topic
- See: https://github.com/paboyle/Grid for code, and also Peter Boyle’s slides from IXPUG: [Here] . Look for 06-Boyle-IXPUG.pdf

Vector Unit of Length N

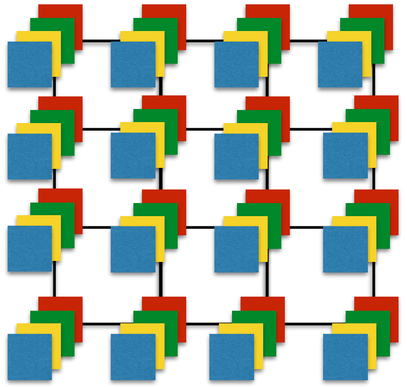
$\log_2 N$ dimensional virtual node grid



Lay-out lattice over virtual node grid



Ascribe corresponding sites from virt. node grid into vector lanes



Extreme Metaprogramming III: QEX

- QEX Project: James Osborn, ALCF, using the Nim language
- Nim (formerly Nimrod) is a very high level language (http://nim-lang.org)
  - generates C/C++, which can then be compiled
    - allows easy integration with C/C++
    - can produce #pragma's in the C-code (OpenMP/OpenACC) intrinsics (SIMD)
    - can interface with C-like languages (CUDA/OpenCL)
  - two levels of metaprogramming
    - use as flexible C/C++ code generator
    - high level AST transformations on any Nim code
  - strongly typed
  - modules: no more arbitraty .h/.cc distinction
  - reflection/introspection: automatic (de)serialization
  - script-like: instead of scripting your executable, have your script be the executable
    - no need to integrate scripting/input language
- Comments:
  - relatively young language
  - would require some infrastructure work (e.g. wrap MPI — Nim provides automatic wrapping tool)
  - very promising initial exploration work
- See http://www.mcs.anl.gov/~osborn/scidac/qex.pdf for details
- QEX code available on GitHub: https://github.com/jcosborn/qex

From J. Osborn's slides: Example Lattice (client) Code

```
import qex
import qcdTypes

qexInit()
var lat = [4,4,4,4]
var lo = newLayout(lat)
var v1 = lo.ColorVector()
var v2 = lo.ColorVector()
var m1 = lo.ColorMatrix()
threads:
  m1 := 1
  v1 := 2
  v2 := m1 * v1
  shift(v1, dir=3, len=1, v2)  # len=+1: from forward
  single:
    if myRank==0:
      echo v2[0][0]  # vector "site" 0, color 0
qexFinalize()
```

Construct Domain Specific Objects

Matrix x Vector
Nearest Neighbors

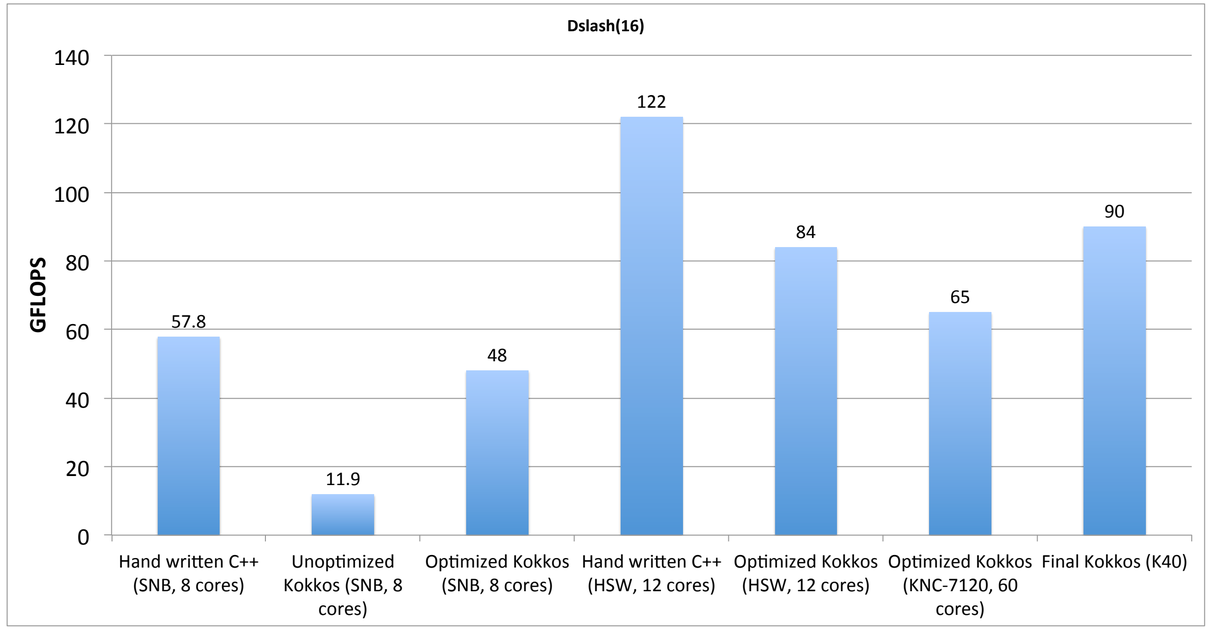
```
template threads*(body:untyped):untyped =
  let tidOld = tid
  let nidOld = nid
  proc tproc =
    {.emit:"#pragma omp parallel".}
    block:
      setupForeignThreadGc()
      tid = ompGetThreadNum()
      nid = ompGetNumThreads()
      body
  tproc()
  tid = tidOld
  nid = nidOld
```

Emit Compiler #pragma

From J. Osborn's slides: Metaprogramming example

Kokkos Experiments

- Kokkos is a programming model for performance portability written in C++
  - many back ends: OpenMP, CUDA, qthreads etc.
- Aesthetically very appealing abstraction of hardware features, and implementation of parallel patterns.
- Initial experiment with a lattice QCD Kernel: $y_i = D\, x_i$ for i=0..15
  - compare Kokkos implementation with a straight C/C++ version. (S. Khan, ODU)
  - Initial performance low (no vectorization)
  - Interaction with Kokkos team (C. Trott) improved performance to over 80% of hand written C++ code
- Big Thanks to Christian Trott from the Kokkos team for optimizing this so promptly!!!
- More work to be done here, hopefully future collaboration with Kokkos team.
- Kokkos is on GitHub: https://github.com/kokkos
  - also, further talks at this workshop: C. Trott, S. Hammond, & others



NB: Optimized = what Christian optimized overnight
Final = what Christian optimized overnight + 1 day
This is not the end, but the beginning (custom layouts etc still to come)

Lessons Learned/Takeaways

- Bespoke High Performance Libraries are extremely valuable but also a real pain
  - High performance, but tied to architecture
  - Low level code, using intrinsics/assembly.
  - Frequently generated by code-generators
  - Complicated algorithms (more complex solvers, force terms) are difficult to implement
    - turn ‘library’ into a ‘framework’ from the bottom-up
  - Feature compatibility often lags between libraries
  - Difficult to maintain
  - Low developer productivity
- Would really like the productive Level 2 frameworks to provide features and performance to remove the need for bespoke libraries
  - performance portability through the performance portability of the framework
  - but potentially decreased reuse for codes using different frameworks (framework dependence)

Lessons Learned/Takeaway: II

- Data layout flexibility and mixed precision algorithms are crucial, especially for memory bandwidth bound problems
- In order to provide ‘expression’ syntax for users, and in order to deal with GPUs as well as CPUs - we had to do to some form of metaprogramming
  - PETE - for QDP++ & QDP-JIT; C++11 improvements for Grid
  - Kokkos uses a lot of metaprogramming under the hood
  - Mixing compile time constructs, with runtime constructs can get very messy.
    - e.g. runtime selection of templated objects
- Nims offers nice features (modules, reflection, scripting etc) and can be used as a high level code-generator for C/C++.
- We’ve not made much use of directives for accelerators so far
  - QUDA library used CUDA since beginning
  - QDP-JIT works at the PTX/LLVM-IR level (depending on implementation)
  - There may be issues using acceleration directives with recursive expression templates.
  - Frameworks should hide this feature from the user.
- Essential to have clean builds, unit tests etc
  - Code is complex (Expression Templates, Low level codes etc), Testing is important. We should always strive to improve software engineering practices.

Acknowledgements

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  - P. Boyle (U. Edinburgh), K. Clark (NVIDIA), R. G. Edwards (JLab), J. Osborn (ANL, ALCF), F. Winter (JLab)
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